

**ABSTRACT**

COMPUTER-AIDED METHOD FOR THE PROVISION, IDENTIFICATION  
AND DESCRIPTION OF MOLECULES CAPABLE OF EXHIBITING A  
5 DESIRED BEHAVIOUR, MORE PARTICULARLY IN THE  
PHARMACEUTICAL SECTOR, AND MOLECULES OBTAINED BY SAID  
METHOD

10 The present invention is concerned with a computer-  
aided method for the provision, identification and  
description of molecules exhibiting a desired behaviour,  
more particularly in the pharmaceutical sector, employing  
a molecular modelling step, a combinatorial library  
15 building step and a step of selecting potentially useful  
molecules, said method including a step whereby the  
candidate molecules are filtered using a dynamic filter  
representing constraints of conformational variations  
which the molecules must satisfy in order to exhibit said  
activity.